

THE HIGH-RESOLUTION ELECTRONIC SPECTRUM OF THE SiCCl FREE RADICAL: PROBING THE CARBON-SILICON TRIPLE BOND

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The 600-515 nm electronic band system of the jet-cooled SiCCl free radical has been studied by laser-induced fluorescence and single vibronic level emission spectroscopy. The radical was produced in an electric discharge through a dilute mixture of 1,1-dichlorosilacyclobutane in high pressure argon. The low-resolution LIF spectrum exhibits bands involving all three excited state vibrations, establishing values for the upper state vibrational frequencies. Emission spectra from thirteen upper state levels yielded the ground state bending and stretching energy levels up to 5000 cm^{-1} . These were satisfactorily fitted to a Renner-Teller model that included spin-orbit and vibrational anharmonicity effects. A high-resolution rotationally resolved spectrum of the $^2\Pi_{3/2}$ spin-orbit component of the 0-0 band was recorded and rotational analysis yielded accurate B values for both states of SiC^{35}Cl and SiC^{37}Cl . These constants were used with fixed *ab initio* C-Cl bond lengths to obtain $r'' = 1.692(1)\text{ \AA}$ and $r' = 1.594(1)\text{ \AA}$. The bond lengths correspond to a silicon-carbon double bond in the ground state and an unusual Si-C triple bond in the excited state, similar to our previous findings for SiCH and SiCF. Halogenation has little effect on the Si-C bond length in both states.